

Optical phonons in the kesterite $\text{Cu}_2\text{ZnGeS}_4$ semiconductor: polarized Raman spectroscopy and first-principle calculations

M. Guc, A. P. Litvinchuk, S. Levchenko, M. Ya. Valakh, I. V. Bodnar, V. M. Dzhagan, V. Izquierdo-Roca, E. Arushanov and A. Pérez-Rodríguez

Supplementary information

Figure S1 shows the X-Ray Diffraction (XRD) measurements that have been performed in a single crystal (red) and in a powder sample that was obtained from single crystal samples that were grown in the same experiment (black). Powder XRD diffractograms were recorded by an X-Pert PRO $\theta/2\theta$ system operated in the Bragg-Bertrano geometry and a copper K-alpha1 ($\text{Cu K}\alpha_1$) line was used as an X-ray source. The normal operating conditions during measurements were 45 kV and 40 mA. Crystal orientation was determined from the measurements from the single crystal sample that were performed on the basal crystal plane using the same XRD system coupled with Goniometer PW3050/65.

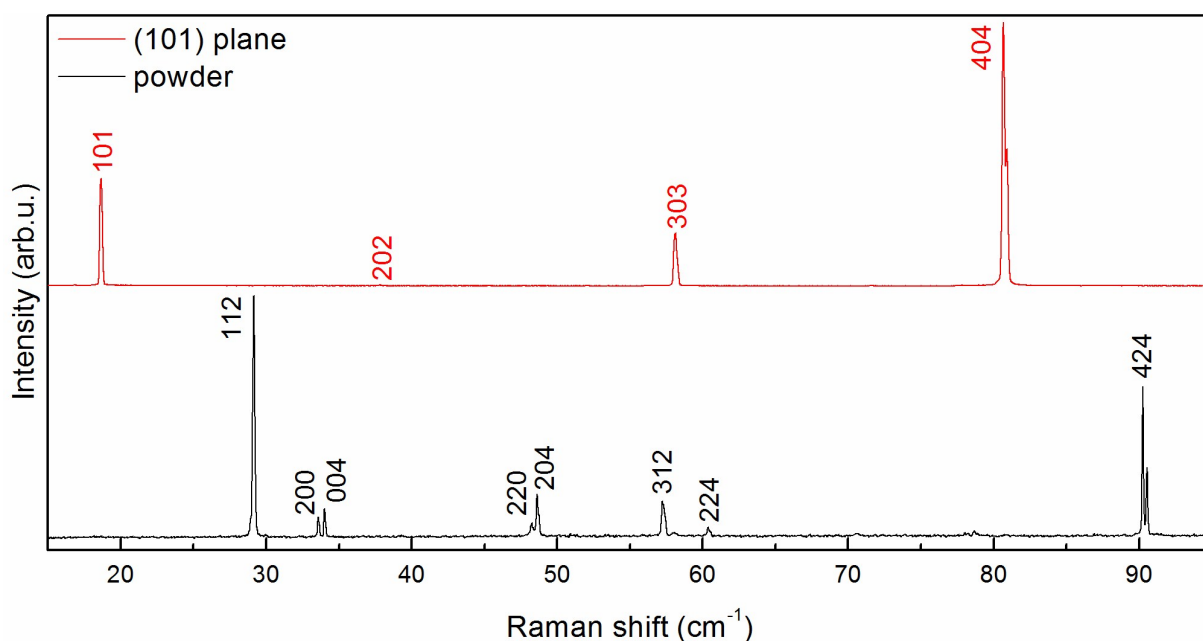


Fig. S1: XRD spectra of $\text{Cu}_2\text{ZnGeS}_4$ measured from (1 0 1) basal plane of single crystal (red) and from powdered samples (black).

XRD spectra from the powdered samples as well as from the crystal basal plane show peaks related only to $\text{Cu}_2\text{ZnGeS}_4$ compound crystalized in tetragonal lattice according to ISCD#152752 file registered in international database.